



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:49 PM UTC

PDB ID : 1YGR / pdb_00001ygr
Title : Crystal structure of the tandem phosphatase domain of RPTP CD45
Authors : Nam, H.J.; Poy, F.; Saito, H.; Frederick, C.A.
Deposited on : 2005-01-05
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

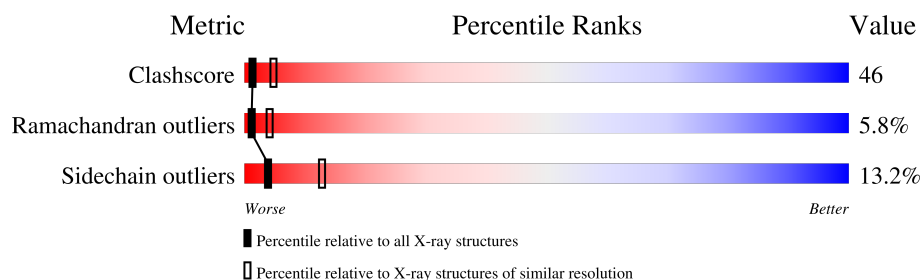
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	610	
1	B	610	
2	C	6	
2	D	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PTR	C	2004	X	-	-	-
2	PTR	D	2004	X	-	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9537 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CD45 Protein Tyrosine Phosphatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	574	Total	C	N	O	S	Se	0	0	0
			4709	2998	821	870	7	13			
1	B	574	Total	C	N	O	S	Se	0	0	0
			4706	2995	820	871	7	13			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	603	MSE	MET	modified residue	UNP P08575
A	627	PRO	LEU	variant	UNP P08575
A	714	MSE	MET	modified residue	UNP P08575
A	725	MSE	MET	modified residue	UNP P08575
A	744	MSE	MET	modified residue	UNP P08575
A	828	SER	CYS	engineered mutation	UNP P08575
A	844	MSE	MET	modified residue	UNP P08575
A	870	MSE	MET	modified residue	UNP P08575
A	907	MSE	MET	modified residue	UNP P08575
A	999	MSE	MET	modified residue	UNP P08575
A	1007	MSE	MET	modified residue	UNP P08575
A	1024	MSE	MET	modified residue	UNP P08575
A	1035	MSE	MET	modified residue	UNP P08575
A	1115	MSE	MET	modified residue	UNP P08575
A	1184	LEU	PRO	variant	UNP P08575
A	1186	MSE	MET	modified residue	UNP P08575
B	603	MSE	MET	modified residue	UNP P08575
B	627	PRO	LEU	variant	UNP P08575
B	714	MSE	MET	modified residue	UNP P08575
B	725	MSE	MET	modified residue	UNP P08575
B	744	MSE	MET	modified residue	UNP P08575
B	828	SER	CYS	engineered mutation	UNP P08575
B	844	MSE	MET	modified residue	UNP P08575
B	870	MSE	MET	modified residue	UNP P08575
B	907	MSE	MET	modified residue	UNP P08575

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Chain	Residue	Modelled	Actual	Comment	Reference
B	999	MSE	MET	modified residue	UNP P08575
B	1007	MSE	MET	modified residue	UNP P08575
B	1024	MSE	MET	modified residue	UNP P08575
B	1035	MSE	MET	modified residue	UNP P08575
B	1115	MSE	MET	modified residue	UNP P08575
B	1184	LEU	PRO	variant	UNP P08575
B	1186	MSE	MET	modified residue	UNP P08575

- Molecule 2 is a protein called T-cell Receptor CD3 zeta ITAM-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	P	0	0	0
			61	34	9	17	1			
2	D	6	Total	C	N	O	P	0	0	0
			61	34	9	17	1			

There are 2 discrepancies between the modelled and reference sequences:

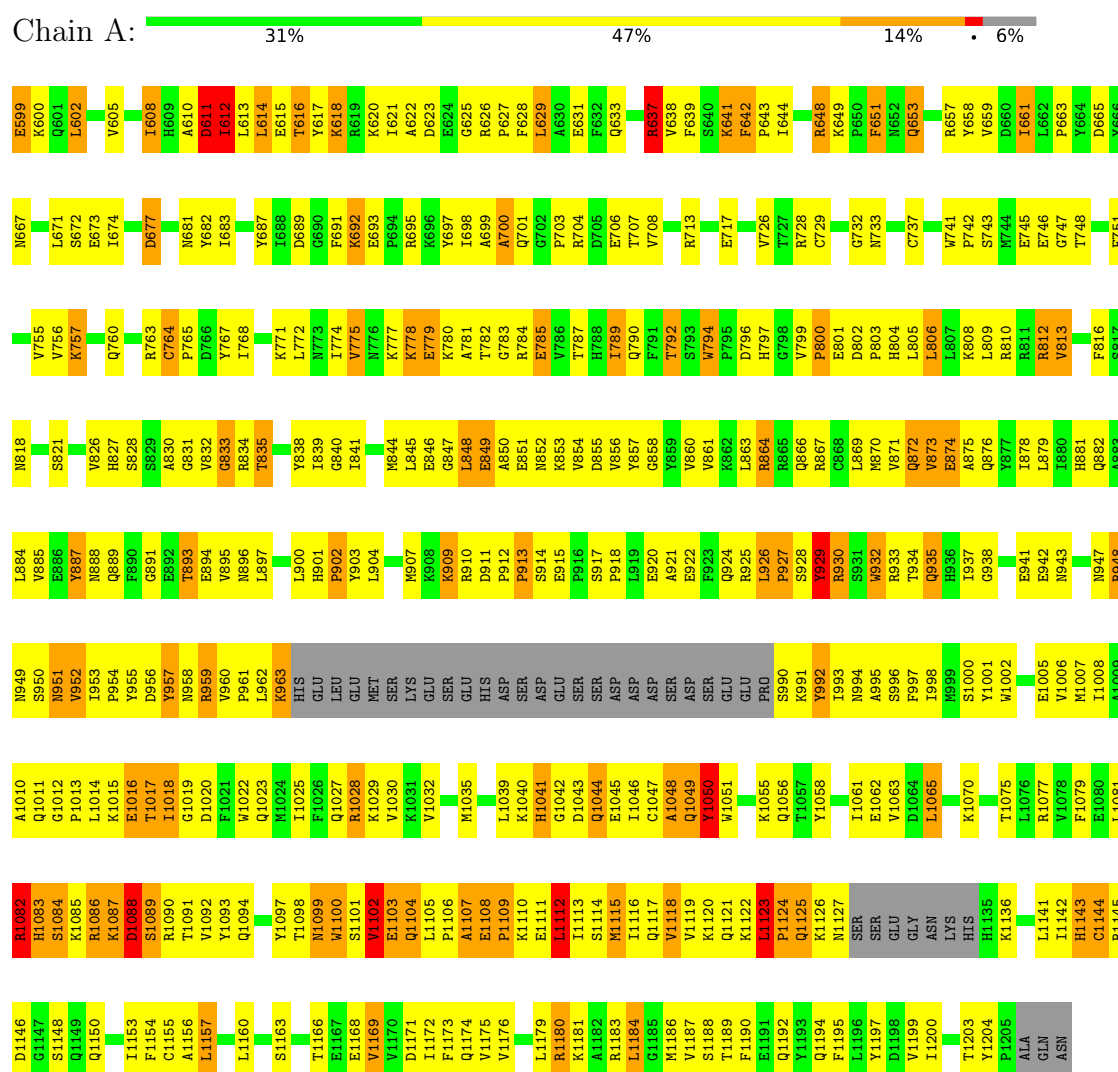
Chain	Residue	Modelled	Actual	Comment	Reference
C	2004	PTR	TYR	modified residue	UNP P20963
D	2004	PTR	TYR	modified residue	UNP P20963

3 Residue-property plots

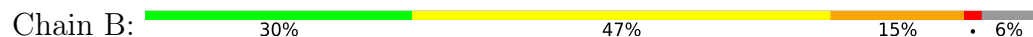
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

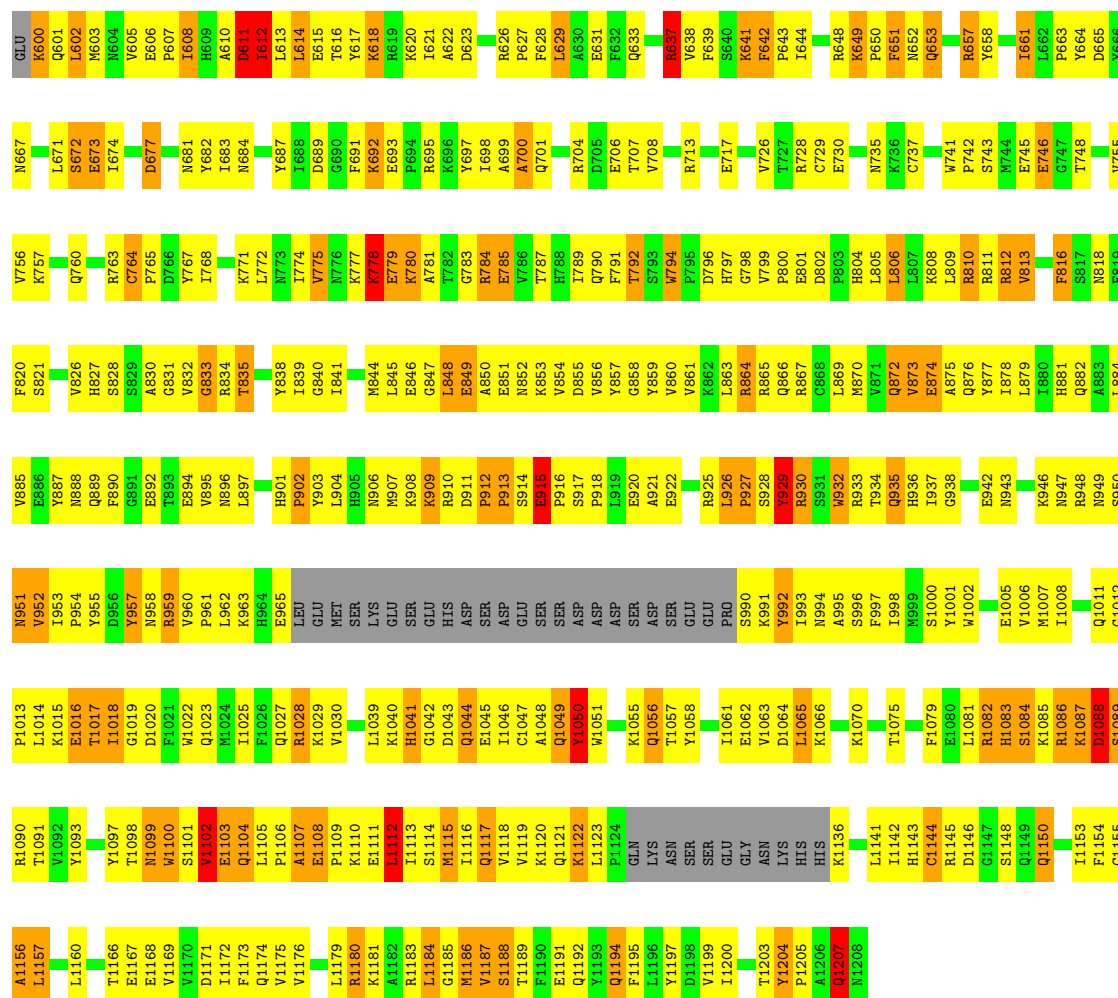
Note EDS was not executed.

• Molecule 1: CD45 Protein Tyrosine Phosphatase



• Molecule 1: CD45 Protein Tyrosine Phosphatase





• Molecule 2: T-cell Receptor CD3 zeta ITAM-1

Chain C: 17% 50% 33%



• Molecule 2: T-cell Receptor CD3 zeta ITAM-1

Chain D: 33% 50% 17%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.01Å 59.70Å 160.53Å 90.00° 99.53° 90.00°	Depositor
Resolution (Å)	29.85 – 2.90	Depositor
% Data completeness (in resolution range)	81.5 (29.85-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.255 , 0.312	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9537	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PTR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/4805	1.07	39/6474 (0.6%)
1	B	0.60	0/4802	1.08	36/6470 (0.6%)
2	C	0.70	0/43	0.68	0/53
2	D	0.77	0/43	0.62	0/53
All	All	0.60	0/9693	1.08	75/13050 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	1	0
2	D	1	0
All	All	2	0

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1112	LEU	N-CA-C	-10.11	100.26	111.28
1	B	1088	ASP	N-CA-C	-9.46	96.53	108.45
1	A	1088	ASP	N-CA-C	-9.24	96.81	108.45
1	A	1112	LEU	N-CA-C	-9.22	101.23	111.28
1	B	887	TYR	N-CA-C	-9.17	101.19	111.82
1	B	778	LYS	N-CA-C	-8.07	102.56	111.36
1	B	649	LYS	CA-C-N	7.36	126.62	118.97
1	B	649	LYS	C-N-CA	7.36	126.62	118.97
1	B	912	PRO	CA-C-N	7.31	128.98	119.84
1	B	912	PRO	C-N-CA	7.31	128.98	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1204	TYR	CA-C-N	6.94	126.98	119.90
1	B	1204	TYR	C-N-CA	6.94	126.98	119.90
1	B	764	CYS	CA-C-N	6.93	128.50	119.84
1	B	764	CYS	C-N-CA	6.93	128.50	119.84
1	A	1108	GLU	CA-C-N	6.83	128.38	119.84
1	A	1108	GLU	C-N-CA	6.83	128.38	119.84
1	A	764	CYS	CA-C-N	6.78	128.32	119.84
1	A	764	CYS	C-N-CA	6.78	128.32	119.84
1	A	992	TYR	N-CA-C	6.62	120.61	109.76
1	A	846	GLU	N-CA-C	-6.54	104.07	111.07
1	B	1108	GLU	CA-C-N	6.42	127.86	119.84
1	B	1108	GLU	C-N-CA	6.42	127.86	119.84
1	A	649	LYS	CA-C-N	6.38	126.13	119.05
1	A	649	LYS	C-N-CA	6.38	126.13	119.05
1	B	665	ASP	N-CA-C	6.31	119.13	111.82
1	A	873	VAL	N-CA-C	6.23	117.67	108.45
1	A	642	PHE	CA-C-N	6.17	126.20	119.90
1	A	642	PHE	C-N-CA	6.17	126.20	119.90
1	A	1123	LEU	N-CA-C	-6.17	101.14	110.39
1	B	700	ALA	N-CA-C	6.15	119.22	109.50
1	A	778	LYS	N-CA-C	-6.15	102.91	110.65
1	B	816	PHE	N-CA-C	6.08	118.38	110.53
1	B	992	TYR	N-CA-C	6.06	119.36	109.06
1	A	661	ILE	N-CA-C	5.94	115.29	106.85
1	A	872	GLN	N-CA-C	5.87	120.18	113.19
1	A	914	SER	N-CA-C	-5.87	106.21	113.19
1	B	1144	CYS	N-CA-C	-5.79	100.76	108.34
1	B	794	TRP	CA-C-N	5.74	125.50	119.76
1	B	794	TRP	C-N-CA	5.74	125.50	119.76
1	A	1144	CYS	N-CA-C	-5.73	100.83	108.34
1	B	846	GLU	N-CA-C	-5.67	104.31	111.11
1	A	849	GLU	N-CA-C	-5.66	105.56	113.37
1	A	1084	SER	N-CA-C	-5.63	106.25	113.01
1	A	812	ARG	N-CA-C	5.60	120.11	113.28
1	B	873	VAL	N-CA-C	5.60	116.74	108.45
1	A	887	TYR	N-CA-C	-5.59	105.26	111.36
1	B	1143	HIS	N-CA-C	5.59	117.59	108.76
1	B	663	PRO	N-CA-C	5.52	119.85	111.19
1	A	781	ALA	N-CA-C	-5.50	100.08	108.76
1	B	813	VAL	N-CA-C	-5.43	104.69	112.35
1	B	1084	SER	N-CA-C	-5.41	106.52	113.01
1	B	642	PHE	CA-C-N	5.37	125.37	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	642	PHE	C-N-CA	5.37	125.37	119.90
1	B	682	TYR	N-CA-C	5.36	118.96	109.96
1	B	810	ARG	N-CA-C	-5.35	105.36	111.14
1	A	789	ILE	CB-CA-C	-5.35	102.68	110.81
1	A	912	PRO	N-CA-C	-5.32	104.21	110.70
1	B	661	ILE	N-CA-C	5.31	114.39	106.85
1	A	665	ASP	N-CA-C	5.28	118.89	112.23
1	A	948	ARG	N-CA-C	-5.24	105.98	112.38
1	A	782	THR	N-CA-C	5.23	118.59	110.17
1	A	616	THR	N-CA-C	-5.20	104.87	111.11
1	A	682	TYR	N-CA-C	5.20	118.28	109.76
1	A	663	PRO	N-CA-C	5.19	119.34	111.19
1	A	700	ALA	N-CA-C	5.18	117.69	109.50
1	B	872	GLN	N-CA-C	5.18	119.36	113.19
1	B	1207	GLN	N-CA-C	5.16	121.79	110.80
1	A	1143	HIS	N-CA-C	5.09	116.99	108.99
1	A	1092	VAL	N-CA-C	5.07	115.15	107.75
1	B	812	ARG	N-CA-C	5.07	119.46	113.28
1	A	794	TRP	CA-C-N	5.06	125.22	119.90
1	A	794	TRP	C-N-CA	5.06	125.22	119.90
1	B	849	GLU	N-CA-C	-5.05	106.39	113.37
1	A	810	ARG	N-CA-C	-5.02	105.72	111.14
1	A	1082	ARG	N-CA-C	5.02	115.16	108.38

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2004	PTR	CA
2	D	2004	PTR	CA

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4709	0	4670	417	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4706	0	4662	450	0
2	C	61	0	43	8	0
2	D	61	0	43	3	0
All	All	9537	0	9418	873	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

All (873) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:TYR:HB3	1:A:932:TRP:HB2	1.22	1.16
1:B:929:TYR:HB3	1:B:932:TRP:HB2	1.23	1.12
1:B:637:ARG:HH11	1:B:637:ARG:HB3	1.07	1.11
1:A:637:ARG:HH11	1:A:637:ARG:HB3	1.09	1.11
1:A:911:ASP:O	1:A:913:PRO:HD3	1.53	1.07
1:B:962:LEU:HD12	1:B:991:LYS:HB2	1.39	1.05
1:B:844:MSE:HE3	1:B:854:VAL:HB	1.43	1.00
1:B:600:LYS:HD3	1:B:600:LYS:N	1.80	0.95
1:B:1183:ARG:HB3	1:B:1186:MSE:HE2	1.49	0.94
1:A:1108:GLU:HB2	1:A:1110:LYS:NZ	1.82	0.93
1:B:911:ASP:HB2	1:B:912:PRO:HD3	1.48	0.92
1:A:929:TYR:HB3	1:A:932:TRP:CB	2.02	0.90
1:B:929:TYR:HD1	1:B:929:TYR:H	1.17	0.90
1:B:952:VAL:HG11	1:B:1146:ASP:HB2	1.53	0.89
1:A:844:MSE:HE3	1:A:854:VAL:HB	1.52	0.89
1:A:775:VAL:HG12	1:A:783:GLY:HA2	1.54	0.88
1:A:889:GLN:HA	1:A:889:GLN:HE21	1.39	0.88
1:A:929:TYR:HD1	1:A:929:TYR:H	1.20	0.88
1:B:929:TYR:HB3	1:B:932:TRP:CB	2.04	0.88
1:A:617:TYR:O	1:A:621:ILE:HG12	1.73	0.88
1:B:844:MSE:HE1	1:B:855:ASP:N	1.89	0.87
1:A:897:LEU:HD12	1:A:1168:GLU:HA	1.56	0.87
1:B:617:TYR:O	1:B:621:ILE:HG12	1.76	0.86
1:B:1108:GLU:HB2	1:B:1110:LYS:NZ	1.91	0.86
1:B:775:VAL:HG12	1:B:783:GLY:CA	2.07	0.85
1:B:942:GLU:HG2	1:B:943:ASN:ND2	1.91	0.85
1:B:954:PRO:HD3	1:B:994:ASN:OD1	1.77	0.85
1:A:775:VAL:HG12	1:A:783:GLY:CA	2.07	0.84
1:A:844:MSE:HE1	1:A:855:ASP:N	1.94	0.83
1:B:1097:TYR:HB2	1:B:1115:MSE:HE2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1022:TRP:HE1	1:B:1050:TYR:HB2	1.45	0.81
1:A:874:GLU:CD	1:A:874:GLU:H	1.88	0.81
1:A:878:ILE:HG22	1:A:882:GLN:HE21	1.46	0.81
1:B:878:ILE:HG22	1:B:882:GLN:HE21	1.44	0.81
1:B:1148:SER:OG	1:B:1183:ARG:HD3	1.80	0.81
1:A:929:TYR:CB	1:A:932:TRP:HB2	2.09	0.80
1:A:942:GLU:HG2	1:A:943:ASN:ND2	1.95	0.80
1:B:874:GLU:CD	1:B:874:GLU:H	1.88	0.80
1:B:1018:ILE:HD11	1:B:1048:ALA:HB1	1.63	0.80
1:A:889:GLN:HA	1:A:889:GLN:NE2	1.95	0.80
1:A:952:VAL:HG11	1:A:1146:ASP:HB2	1.63	0.80
1:A:873:VAL:HG12	1:A:875:ALA:H	1.46	0.79
1:A:909:LYS:HD2	1:A:909:LYS:C	2.06	0.79
1:B:1023:GLN:O	1:B:1027:GLN:HG3	1.81	0.79
1:B:1070:LYS:HG2	1:B:1075:THR:HG22	1.65	0.79
1:A:1023:GLN:O	1:A:1027:GLN:HG3	1.83	0.79
1:A:809:LEU:O	1:A:813:VAL:HG13	1.83	0.79
1:B:873:VAL:HG12	1:B:875:ALA:H	1.47	0.79
1:B:637:ARG:HH11	1:B:637:ARG:CB	1.93	0.78
1:B:637:ARG:HB3	1:B:637:ARG:NH1	1.93	0.78
1:B:794:TRP:CZ3	1:B:806:LEU:HD11	2.18	0.77
2:C:2006:VAL:OXT	2:C:2006:VAL:HG12	1.84	0.77
1:A:1018:ILE:HD11	1:A:1048:ALA:HB1	1.66	0.77
1:B:775:VAL:HG12	1:B:783:GLY:HA3	1.66	0.77
1:A:1142:ILE:HD13	1:A:1154:PHE:HD2	1.50	0.77
1:B:1142:ILE:HD13	1:B:1154:PHE:HD2	1.50	0.77
1:A:794:TRP:CZ3	1:A:806:LEU:HD11	2.20	0.77
1:A:659:VAL:HG11	2:C:2001:ARG:HH11	1.48	0.76
1:A:1022:TRP:HE1	1:A:1050:TYR:HB2	1.49	0.76
1:B:673:GLU:HG2	1:B:681:ASN:HB3	1.68	0.76
1:A:637:ARG:HH11	1:A:637:ARG:CB	1.96	0.75
1:B:1160:LEU:CD2	1:B:1175:VAL:HG21	2.16	0.75
1:B:884:LEU:O	1:B:888:ASN:HB2	1.87	0.75
1:B:929:TYR:CB	1:B:932:TRP:HB2	2.11	0.75
1:A:673:GLU:HG2	1:A:681:ASN:HB3	1.66	0.75
1:A:638:VAL:HG12	1:A:639:PHE:H	1.51	0.75
1:B:809:LEU:O	1:B:813:VAL:HG13	1.87	0.75
2:C:2001:ARG:O	2:C:2002:GLU:HB2	1.84	0.75
1:A:637:ARG:HB3	1:A:637:ARG:NH1	1.95	0.75
1:A:929:TYR:HD2	1:A:932:TRP:CD1	2.05	0.74
1:A:1160:LEU:CD2	1:A:1175:VAL:HG21	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:VAL:HG12	1:B:639:PHE:H	1.53	0.74
1:A:614:LEU:HB3	1:A:615:GLU:OE2	1.87	0.74
1:A:631:GLU:O	1:A:857:TYR:HE1	1.71	0.74
1:A:1022:TRP:CZ3	1:A:1025:ILE:HD11	2.23	0.74
1:B:605:VAL:HG21	1:B:857:TYR:HB3	1.70	0.74
1:A:1108:GLU:HB2	1:A:1110:LYS:HZ3	1.50	0.73
1:A:1088:ASP:O	1:A:1089:SER:HB2	1.86	0.73
1:B:929:TYR:CE2	1:B:1181:LYS:HG3	2.23	0.73
1:B:929:TYR:N	1:B:929:TYR:CD1	2.56	0.73
1:B:1088:ASP:O	1:B:1089:SER:HB2	1.87	0.73
1:A:659:VAL:HG11	2:C:2001:ARG:NH1	2.03	0.73
1:A:612:ILE:HA	1:A:615:GLU:OE1	1.88	0.73
1:A:895:VAL:HG21	1:A:900:LEU:HA	1.71	0.73
1:B:918:PRO:O	1:B:921:ALA:HB3	1.89	0.73
1:B:614:LEU:HB3	1:B:615:GLU:OE2	1.89	0.72
1:B:620:LYS:HE3	1:B:631:GLU:OE1	1.89	0.72
1:B:927:PRO:HB2	1:B:929:TYR:CE1	2.23	0.72
1:B:826:VAL:HG12	1:B:835:THR:HB	1.72	0.72
1:A:929:TYR:N	1:A:929:TYR:CD1	2.58	0.72
1:B:1108:GLU:HB2	1:B:1110:LYS:HZ3	1.53	0.72
1:B:960:VAL:HG23	1:B:995:ALA:O	1.91	0.71
1:A:1097:TYR:HB2	1:A:1115:MSE:HE2	1.69	0.71
1:B:1153:ILE:HD11	1:B:1192:GLN:HB3	1.72	0.71
1:A:938:GLY:HA3	1:A:953:ILE:HG21	1.71	0.71
1:B:948:ARG:HH12	1:B:1045:GLU:HG3	1.54	0.71
1:B:1070:LYS:HG2	1:B:1075:THR:CG2	2.20	0.71
1:B:1087:LYS:H	1:B:1087:LYS:HE3	1.56	0.71
1:A:1082:ARG:HB3	1:A:1082:ARG:NH1	2.05	0.71
1:A:1020:ASP:HA	1:A:1023:GLN:OE1	1.91	0.70
1:A:863:LEU:HD22	1:A:870:MSE:HE2	1.74	0.70
1:A:1098:THR:O	1:A:1100:TRP:N	2.24	0.70
1:B:775:VAL:HG12	1:B:783:GLY:HA2	1.74	0.70
1:B:789:ILE:HD11	1:B:816:PHE:CE2	2.26	0.70
1:B:605:VAL:HG21	1:B:857:TYR:CB	2.21	0.70
1:A:787:THR:HG21	1:A:816:PHE:CD2	2.27	0.69
1:A:927:PRO:HB2	1:A:929:TYR:CE1	2.27	0.69
1:B:906:ASN:HB3	1:B:909:LYS:NZ	2.06	0.69
1:B:909:LYS:HD2	1:B:909:LYS:O	1.92	0.69
1:B:1020:ASP:HA	1:B:1023:GLN:OE1	1.92	0.69
1:A:962:LEU:HD12	1:A:993:ILE:HB	1.73	0.69
1:B:955:TYR:OH	1:B:1184:LEU:HD23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:PRO:O	1:A:921:ALA:HB3	1.94	0.68
1:A:600:LYS:N	1:A:600:LYS:HD2	2.08	0.68
1:A:938:GLY:HA3	1:A:953:ILE:CG2	2.22	0.68
1:B:813:VAL:HG21	1:B:838:TYR:OH	1.94	0.68
1:B:951:ASN:N	1:B:951:ASN:HD22	1.89	0.68
1:B:1098:THR:O	1:B:1100:TRP:N	2.25	0.68
1:B:926:LEU:HG	1:B:1173:PHE:CE1	2.28	0.68
1:B:700:ALA:O	1:B:827:HIS:HB2	1.93	0.68
1:B:1180:ARG:HG2	1:B:1180:ARG:HH11	1.58	0.68
1:A:1061:ILE:HD12	1:A:1061:ILE:O	1.94	0.68
1:A:894:GLU:HG3	1:A:1171:ASP:HB2	1.76	0.67
1:A:881:HIS:O	1:A:885:VAL:HG23	1.95	0.67
1:A:948:ARG:HH12	1:A:1045:GLU:HG3	1.59	0.67
1:B:1061:ILE:HD12	1:B:1061:ILE:C	2.20	0.67
1:B:805:LEU:O	1:B:808:LYS:HB3	1.93	0.67
1:B:1160:LEU:HD23	1:B:1175:VAL:HG21	1.76	0.67
1:B:608:ILE:HD12	1:B:608:ILE:H	1.60	0.67
1:B:1011:GLN:HB2	1:B:1145:ARG:O	1.95	0.67
1:B:1118:VAL:O	1:B:1121:GLN:HG2	1.95	0.67
1:B:631:GLU:O	1:B:857:TYR:HE1	1.78	0.66
1:B:808:LYS:HE2	1:B:894:GLU:OE2	1.96	0.66
1:A:1011:GLN:HB2	1:A:1145:ARG:O	1.95	0.66
1:A:929:TYR:CD2	1:A:932:TRP:CD1	2.83	0.66
1:B:1022:TRP:CZ3	1:B:1025:ILE:HD11	2.30	0.66
1:A:620:LYS:HE3	1:A:631:GLU:OE1	1.96	0.66
1:B:864:ARG:HE	1:B:869:LEU:HA	1.59	0.66
1:B:885:VAL:O	1:B:888:ASN:HB3	1.95	0.66
1:A:667:ASN:O	1:A:687:TYR:HD1	1.79	0.65
1:A:743:SER:OG	1:A:746:GLU:HG3	1.95	0.65
1:B:1061:ILE:HD12	1:B:1061:ILE:O	1.97	0.65
1:A:700:ALA:O	1:A:827:HIS:HB2	1.97	0.65
1:B:789:ILE:HD11	1:B:816:PHE:HE2	1.61	0.65
1:B:844:MSE:HE2	1:B:856:VAL:N	2.11	0.65
1:B:951:ASN:N	1:B:951:ASN:ND2	2.44	0.65
1:A:608:ILE:HD12	1:A:608:ILE:H	1.61	0.65
1:A:1087:LYS:HE3	1:A:1087:LYS:H	1.62	0.65
1:B:960:VAL:HG22	1:B:997:PHE:CD2	2.32	0.65
1:A:1061:ILE:HD12	1:A:1061:ILE:C	2.22	0.65
1:B:844:MSE:CE	1:B:854:VAL:HB	2.23	0.65
1:B:962:LEU:HB2	1:B:991:LYS:HG2	1.78	0.65
1:A:1046:ILE:HG23	1:A:1145:ARG:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:TYR:O	1:A:861:VAL:HG23	1.96	0.64
1:A:599:GLU:C	1:A:600:LYS:HD2	2.23	0.64
1:A:960:VAL:HG23	1:A:995:ALA:O	1.97	0.64
1:A:1070:LYS:HG2	1:A:1075:THR:HG22	1.78	0.64
1:A:1153:ILE:HD11	1:A:1192:GLN:HB3	1.80	0.64
1:B:1007:MSE:CE	1:B:1155:CYS:SG	2.85	0.64
1:A:1082:ARG:HD2	1:A:1086:ARG:HA	1.78	0.64
1:A:926:LEU:HG	1:A:1173:PHE:CE1	2.33	0.64
1:B:1101:SER:C	1:B:1103:GLU:H	2.05	0.64
1:B:929:TYR:HD1	1:B:929:TYR:N	1.91	0.63
1:B:933:ARG:HG2	1:B:934:THR:H	1.63	0.63
1:A:1160:LEU:HD23	1:A:1175:VAL:HG21	1.78	0.63
1:B:828:SER:HB3	1:B:835:THR:HG22	1.80	0.63
1:B:927:PRO:HB2	1:B:929:TYR:HE1	1.62	0.63
1:A:805:LEU:O	1:A:808:LYS:HB3	1.98	0.63
1:A:1183:ARG:HB3	1:A:1186:MSE:HE2	1.80	0.63
1:B:1112:LEU:HD12	1:B:1116:ILE:HD11	1.81	0.63
1:B:873:VAL:HG12	1:B:875:ALA:N	2.13	0.63
1:A:704:ARG:H	1:A:707:THR:HB	1.63	0.63
1:A:933:ARG:HG2	1:A:934:THR:H	1.63	0.63
1:A:1114:SER:O	1:A:1118:VAL:HG12	1.98	0.63
1:A:889:GLN:NE2	1:A:889:GLN:CA	2.62	0.63
1:B:608:ILE:HD12	1:B:608:ILE:N	2.13	0.63
1:A:933:ARG:HG2	1:A:934:THR:N	2.14	0.63
1:A:605:VAL:HG21	1:A:857:TYR:HB3	1.80	0.63
1:A:826:VAL:HG12	1:A:835:THR:HB	1.81	0.62
1:B:933:ARG:HG2	1:B:934:THR:N	2.12	0.62
1:A:1124:PRO:O	1:A:1125:GLN:HB2	1.98	0.62
1:A:1115:MSE:O	1:A:1119:VAL:HG23	2.00	0.62
1:A:831:GLY:HA2	1:A:835:THR:HG21	1.81	0.62
1:A:1083:HIS:ND1	1:A:1085:LYS:HB3	2.14	0.62
1:B:629:LEU:O	1:B:633:GLN:HB2	1.99	0.62
1:B:785:GLU:H	1:B:785:GLU:CD	2.07	0.62
1:B:1186:MSE:C	1:B:1188:SER:H	2.07	0.62
1:A:726:VAL:HG12	1:A:726:VAL:O	1.99	0.62
1:B:1108:GLU:O	1:B:1111:GLU:HG2	2.00	0.62
1:A:1002:TRP:HZ2	1:A:1166:THR:HG21	1.64	0.62
1:A:1014:LEU:O	1:A:1016:GLU:N	2.32	0.62
1:A:778:LYS:O	1:A:779:GLU:HB2	2.00	0.61
1:B:831:GLY:HA2	1:B:835:THR:HG21	1.82	0.61
1:A:785:GLU:CD	1:A:785:GLU:H	2.07	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:ILE:O	1:A:1176:VAL:HG23	2.01	0.61
1:B:641:LYS:HG2	1:B:642:PHE:H	1.65	0.61
1:B:1082:ARG:NH1	1:B:1082:ARG:HB3	2.16	0.61
1:A:1040:LYS:HB3	1:A:1045:GLU:HA	1.82	0.61
1:B:811:ARG:HD2	1:B:892:GLU:OE2	1.99	0.61
1:A:1180:ARG:HH11	1:A:1180:ARG:HG2	1.65	0.61
1:B:910:ARG:HD3	1:B:915:GLU:O	2.00	0.61
1:B:873:VAL:HB	1:B:876:GLN:HG3	1.81	0.61
1:A:608:ILE:HD12	1:A:608:ILE:N	2.16	0.61
1:A:813:VAL:HG21	1:A:838:TYR:OH	2.01	0.61
1:A:1113:ILE:HG13	1:A:1203:THR:HG21	1.82	0.61
1:A:929:TYR:HD1	1:A:929:TYR:N	1.95	0.61
1:A:818:ASN:ND2	1:A:821:SER:HA	2.15	0.61
1:A:889:GLN:HE21	1:A:889:GLN:CA	2.07	0.61
1:A:1118:VAL:O	1:A:1121:GLN:HG2	2.00	0.61
1:A:818:ASN:HD21	1:A:821:SER:HA	1.65	0.61
1:A:848:LEU:C	1:A:850:ALA:H	2.07	0.60
1:A:760:GLN:HB2	1:A:771:LYS:HB2	1.83	0.60
1:A:806:LEU:HD23	1:A:841:ILE:HD11	1.81	0.60
1:B:602:LEU:H	1:B:602:LEU:HD22	1.67	0.60
1:B:704:ARG:H	1:B:707:THR:HB	1.66	0.60
1:B:1101:SER:O	1:B:1103:GLU:N	2.34	0.60
1:B:1186:MSE:O	1:B:1188:SER:N	2.34	0.60
1:B:687:TYR:HB3	1:B:695:ARG:HG2	1.83	0.60
1:B:848:LEU:C	1:B:850:ALA:H	2.08	0.60
1:A:991:LYS:HG2	1:A:992:TYR:H	1.67	0.60
1:A:1183:ARG:HB3	1:A:1186:MSE:CE	2.31	0.60
1:B:960:VAL:HG22	1:B:997:PHE:CE2	2.37	0.60
1:B:990:SER:C	1:B:991:LYS:HD3	2.26	0.60
1:A:812:ARG:HG2	1:A:812:ARG:HH11	1.65	0.60
1:A:1070:LYS:HG2	1:A:1075:THR:CG2	2.31	0.60
1:B:818:ASN:ND2	1:B:821:SER:HA	2.17	0.60
1:A:802:ASP:OD2	1:A:804:HIS:HB3	2.02	0.60
1:A:1002:TRP:CZ2	1:A:1166:THR:HG21	2.37	0.60
1:B:929:TYR:HD2	1:B:932:TRP:CD1	2.20	0.60
1:B:1014:LEU:O	1:B:1016:GLU:N	2.35	0.60
1:B:1022:TRP:NE1	1:B:1050:TYR:HB2	2.15	0.60
1:B:1043:ASP:OD1	1:B:1044:GLN:NE2	2.35	0.60
1:B:1088:ASP:CG	1:B:1089:SER:N	2.60	0.60
1:B:1039:LEU:HD22	1:B:1049:GLN:HG3	1.84	0.59
1:A:951:ASN:N	1:A:951:ASN:ND2	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:906:ASN:C	1:B:908:LYS:N	2.58	0.59
1:B:907:MSE:HE2	1:B:922:GLU:OE1	2.03	0.59
1:B:1040:LYS:HB3	1:B:1045:GLU:HA	1.84	0.59
1:B:667:ASN:O	1:B:687:TYR:HD1	1.85	0.59
1:B:1184:LEU:HD13	1:B:1185:GLY:H	1.68	0.59
1:A:626:ARG:N	1:A:627:PRO:CD	2.65	0.59
1:A:927:PRO:HB2	1:A:929:TYR:HE1	1.68	0.59
1:A:605:VAL:HG21	1:A:857:TYR:CB	2.32	0.59
1:A:929:TYR:CE2	1:A:1181:LYS:HG3	2.37	0.59
1:B:897:LEU:HD12	1:B:1168:GLU:HB3	1.83	0.59
1:A:1039:LEU:HD22	1:A:1048:ALA:O	2.03	0.59
1:A:1160:LEU:HD21	1:A:1175:VAL:HG21	1.84	0.59
1:A:844:MSE:HE2	1:A:856:VAL:N	2.18	0.59
1:B:1039:LEU:HD22	1:B:1048:ALA:O	2.02	0.59
1:A:951:ASN:N	1:A:951:ASN:HD22	2.01	0.59
1:A:1022:TRP:NE1	1:A:1050:TYR:HB2	2.17	0.58
1:B:938:GLY:HA3	1:B:953:ILE:HG21	1.85	0.58
1:B:881:HIS:O	1:B:885:VAL:HG23	2.03	0.58
1:B:1113:ILE:HG13	1:B:1203:THR:HG21	1.83	0.58
1:A:800:PRO:HD2	1:A:879:LEU:HD11	1.85	0.58
1:B:1186:MSE:C	1:B:1188:SER:N	2.62	0.58
1:A:933:ARG:CG	1:A:934:THR:H	2.16	0.58
1:B:1087:LYS:HE3	1:B:1087:LYS:N	2.18	0.58
1:A:960:VAL:HG13	1:A:997:PHE:HE2	1.67	0.58
1:B:906:ASN:C	1:B:908:LYS:H	2.10	0.58
1:B:612:ILE:HA	1:B:615:GLU:OE1	2.03	0.58
1:B:938:GLY:HA3	1:B:953:ILE:CG2	2.33	0.58
1:A:844:MSE:CE	1:A:854:VAL:HB	2.30	0.57
1:A:873:VAL:HG12	1:A:875:ALA:N	2.18	0.57
1:B:626:ARG:N	1:B:627:PRO:CD	2.67	0.57
1:B:929:TYR:CD2	1:B:932:TRP:CD1	2.92	0.57
1:B:1008:ILE:HB	1:B:1141:LEU:HG	1.85	0.57
1:A:1082:ARG:CD	1:A:1086:ARG:HA	2.34	0.57
1:B:789:ILE:CD1	1:B:813:VAL:HG12	2.33	0.57
1:B:1099:ASN:O	1:B:1100:TRP:HB2	2.03	0.57
1:B:1115:MSE:O	1:B:1119:VAL:HG23	2.03	0.57
1:A:687:TYR:HB3	1:A:695:ARG:HG2	1.87	0.57
1:A:1148:SER:OG	1:A:1183:ARG:HD3	2.05	0.57
1:A:729:CYS:HB3	1:A:737:CYS:O	2.04	0.57
1:A:932:TRP:HZ3	1:A:957:TYR:CE2	2.23	0.57
1:A:756:VAL:CG1	1:A:772:LEU:HD23	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1088:ASP:CG	1:A:1089:SER:N	2.63	0.57
1:B:800:PRO:HD2	1:B:879:LEU:HD11	1.87	0.57
1:A:869:LEU:HD21	2:C:2005:ASP:HB2	1.86	0.57
1:A:629:LEU:O	1:A:633:GLN:HB2	2.05	0.57
1:B:756:VAL:CG1	1:B:772:LEU:HD23	2.34	0.57
1:B:802:ASP:OD2	1:B:804:HIS:HB3	2.03	0.57
1:B:841:ILE:HG22	1:B:845:LEU:HD11	1.85	0.57
1:B:1160:LEU:HD21	1:B:1175:VAL:HG21	1.85	0.57
1:B:1180:ARG:HG2	1:B:1180:ARG:NH1	2.18	0.57
1:A:741:TRP:HB2	1:A:742:PRO:HD2	1.87	0.57
1:B:910:ARG:NH1	1:B:916:PRO:HA	2.20	0.57
1:B:951:ASN:ND2	1:B:951:ASN:H	2.03	0.57
1:A:993:ILE:HG23	1:A:993:ILE:O	2.04	0.56
1:B:1105:LEU:O	1:B:1106:PRO:C	2.47	0.56
1:B:1187:VAL:O	1:B:1189:THR:N	2.36	0.56
1:A:641:LYS:HG2	1:A:642:PHE:H	1.70	0.56
1:A:1105:LEU:O	1:A:1106:PRO:C	2.48	0.56
1:A:631:GLU:HG2	1:A:857:TYR:CD1	2.40	0.56
1:A:942:GLU:OE1	1:A:942:GLU:N	2.38	0.56
1:A:955:TYR:OH	1:A:1184:LEU:HD23	2.05	0.56
1:A:1112:LEU:HD12	1:A:1116:ILE:HD11	1.86	0.56
1:B:614:LEU:O	1:B:618:LYS:HG2	2.05	0.56
1:B:692:LYS:O	1:B:693:GLU:C	2.49	0.56
1:B:789:ILE:CD1	1:B:816:PHE:HE2	2.18	0.56
1:B:996:SER:HB2	1:B:1183:ARG:HE	1.68	0.56
1:A:1077:ARG:HE	1:A:1094:GLN:HE22	1.54	0.56
1:B:1112:LEU:O	1:B:1116:ILE:HG13	2.04	0.56
1:A:1007:MSE:CE	1:A:1155:CYS:SG	2.94	0.56
1:A:767:TYR:OH	1:A:812:ARG:HD3	2.05	0.56
1:A:789:ILE:HG12	1:A:816:PHE:HE2	1.70	0.56
1:A:913:PRO:C	1:A:915:GLU:H	2.11	0.56
1:B:764:CYS:HB3	1:B:765:PRO:HD2	1.88	0.56
1:B:851:GLU:HB2	1:B:853:LYS:HG2	1.88	0.56
1:B:906:ASN:HA	1:B:909:LYS:HG3	1.87	0.56
1:B:929:TYR:HE2	1:B:1181:LYS:NZ	2.03	0.56
1:A:617:TYR:CE2	1:A:621:ILE:HD13	2.41	0.56
1:A:767:TYR:HA	1:A:790:GLN:O	2.05	0.56
1:B:689:ASP:H	1:B:866:GLN:HE22	1.54	0.56
1:B:704:ARG:HH21	1:B:706:GLU:CD	2.14	0.56
1:B:704:ARG:NH2	1:B:706:GLU:OE2	2.35	0.56
1:B:855:ASP:OD2	1:B:858:GLY:HA3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:933:ARG:CG	1:B:934:THR:H	2.19	0.56
1:B:1028:ARG:HH22	1:B:1136:LYS:NZ	2.03	0.56
1:B:1083:HIS:ND1	1:B:1085:LYS:HB3	2.21	0.56
1:A:1022:TRP:CE3	1:A:1025:ILE:HD11	2.40	0.55
1:A:1055:LYS:HE3	1:A:1062:GLU:CD	2.31	0.55
1:A:1082:ARG:HB3	1:A:1082:ARG:HH11	1.71	0.55
1:B:767:TYR:OH	1:B:812:ARG:HD3	2.06	0.55
1:A:1014:LEU:C	1:A:1016:GLU:H	2.13	0.55
1:B:961:PRO:HB2	1:B:963:LYS:HE2	1.88	0.55
1:A:1101:SER:C	1:A:1103:GLU:H	2.15	0.55
1:B:1083:HIS:ND1	1:B:1083:HIS:N	2.54	0.55
1:B:863:LEU:HD22	1:B:870:MSE:HE2	1.87	0.55
1:A:1040:LYS:CB	1:A:1045:GLU:HA	2.36	0.55
1:B:784:ARG:HD2	1:B:820:PHE:CZ	2.41	0.55
1:B:1013:PRO:HD2	1:B:1047:CYS:SG	2.47	0.55
1:B:1014:LEU:C	1:B:1016:GLU:H	2.13	0.55
1:B:1007:MSE:HE1	1:B:1155:CYS:HA	1.89	0.55
1:B:812:ARG:HH11	1:B:812:ARG:HG2	1.70	0.55
1:A:1180:ARG:HG2	1:A:1180:ARG:NH1	2.22	0.55
1:B:1114:SER:O	1:B:1118:VAL:HG12	2.06	0.55
1:A:929:TYR:HB3	1:A:932:TRP:CG	2.41	0.54
1:A:1028:ARG:HG3	1:A:1028:ARG:HH11	1.72	0.54
1:B:611:ASP:OD1	1:B:612:ILE:HG23	2.06	0.54
1:B:797:HIS:CD2	1:B:872:GLN:HE22	2.25	0.54
1:B:996:SER:N	1:B:1183:ARG:HH21	2.05	0.54
1:B:998:ILE:O	1:B:1006:VAL:HG13	2.07	0.54
1:B:1200:ILE:O	1:B:1204:TYR:HB2	2.07	0.54
1:A:960:VAL:HG22	1:A:997:PHE:CD2	2.41	0.54
1:A:1183:ARG:CB	1:A:1186:MSE:HE2	2.37	0.54
1:A:611:ASP:OD1	1:A:612:ILE:HG23	2.08	0.54
1:A:864:ARG:HE	1:A:869:LEU:HA	1.72	0.54
1:B:1018:ILE:HD11	1:B:1048:ALA:CB	2.35	0.54
1:B:993:ILE:CG1	1:B:994:ASN:N	2.71	0.54
1:B:1120:LYS:HA	1:B:1123:LEU:HD12	1.89	0.54
1:A:960:VAL:HG13	1:A:997:PHE:CE2	2.42	0.54
1:A:1041:HIS:ND1	1:A:1041:HIS:C	2.65	0.54
1:A:1087:LYS:HE3	1:A:1087:LYS:N	2.21	0.54
1:B:600:LYS:N	1:B:600:LYS:CD	2.54	0.54
1:B:743:SER:OG	1:B:746:GLU:HG3	2.08	0.54
1:B:794:TRP:NE1	1:B:834:ARG:HG2	2.23	0.54
1:B:1102:VAL:HG11	1:B:1145:ARG:NE	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:760:GLN:HB2	1:B:771:LYS:HB2	1.90	0.54
1:A:644:ILE:O	1:A:644:ILE:HG22	2.08	0.53
1:A:775:VAL:HG12	1:A:783:GLY:HA3	1.86	0.53
1:B:960:VAL:HG13	1:B:997:PHE:HE2	1.73	0.53
1:A:907:MSE:HE2	1:A:922:GLU:OE1	2.09	0.53
1:B:906:ASN:HB3	1:B:909:LYS:HZ3	1.72	0.53
1:A:856:VAL:O	1:A:857:TYR:C	2.52	0.53
1:A:1035:MSE:HG3	1:A:1143:HIS:CE1	2.44	0.53
1:B:1030:VAL:HG21	1:B:1141:LEU:HD12	1.89	0.53
1:B:1063:VAL:HG12	1:B:1081:LEU:HD22	1.89	0.53
1:A:1083:HIS:CE1	1:A:1085:LYS:HB3	2.43	0.53
1:B:691:PHE:CZ	1:B:847:GLY:HA2	2.44	0.53
1:B:844:MSE:HE2	1:B:856:VAL:CA	2.39	0.53
1:A:794:TRP:NE1	1:A:834:ARG:HG2	2.24	0.53
1:A:704:ARG:HH21	1:A:706:GLU:CD	2.16	0.53
1:A:1007:MSE:HE1	1:A:1155:CYS:HA	1.91	0.53
1:A:1100:TRP:CE2	1:A:1106:PRO:HG3	2.43	0.53
1:B:808:LYS:HE2	1:B:894:GLU:CD	2.33	0.53
1:A:933:ARG:CG	1:A:934:THR:N	2.72	0.53
1:A:1013:PRO:HD2	1:A:1047:CYS:SG	2.48	0.53
1:B:657:ARG:HH12	1:B:704:ARG:HA	1.74	0.53
1:B:1082:ARG:HD2	1:B:1086:ARG:HA	1.91	0.53
2:C:2006:VAL:OXT	2:C:2006:VAL:CG1	2.57	0.53
1:A:911:ASP:C	1:A:913:PRO:HD3	2.28	0.53
1:B:614:LEU:HD21	1:B:889:GLN:OE1	2.09	0.53
1:B:1014:LEU:C	1:B:1016:GLU:N	2.67	0.53
1:B:1040:LYS:CB	1:B:1045:GLU:HA	2.38	0.53
1:B:1187:VAL:C	1:B:1189:THR:H	2.16	0.53
1:A:704:ARG:NH2	1:A:706:GLU:OE2	2.39	0.53
1:A:1108:GLU:O	1:A:1111:GLU:HG2	2.09	0.53
1:B:1002:TRP:CZ2	1:B:1166:THR:HG21	2.44	0.53
1:A:789:ILE:CD1	1:A:813:VAL:HG12	2.39	0.53
1:A:962:LEU:HD11	1:A:1020:ASP:HB3	1.91	0.53
1:A:1112:LEU:O	1:A:1116:ILE:HG13	2.09	0.52
1:B:857:TYR:O	1:B:861:VAL:HG23	2.08	0.52
1:B:1055:LYS:HE3	1:B:1062:GLU:CD	2.33	0.52
1:B:1083:HIS:CE1	1:B:1085:LYS:HB3	2.44	0.52
1:B:1171:ASP:OD1	1:B:1174:GLN:HB2	2.09	0.52
1:A:764:CYS:HB3	1:A:765:PRO:HD2	1.91	0.52
1:A:895:VAL:HG22	1:A:896:ASN:N	2.24	0.52
1:A:909:LYS:HD2	1:A:909:LYS:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:VAL:O	1:B:726:VAL:HG12	2.08	0.52
1:A:789:ILE:HD11	1:A:816:PHE:CE2	2.45	0.52
1:B:631:GLU:HG2	1:B:857:TYR:CD1	2.44	0.52
1:B:932:TRP:HZ3	1:B:957:TYR:CE2	2.27	0.52
1:B:806:LEU:O	1:B:809:LEU:HD23	2.10	0.52
1:B:874:GLU:O	1:B:878:ILE:HG13	2.09	0.52
1:B:1000:SER:HB3	1:B:1005:GLU:O	2.10	0.52
1:B:1046:ILE:HG23	1:B:1145:ARG:HG2	1.89	0.52
1:B:1100:TRP:CE2	1:B:1106:PRO:HG3	2.45	0.52
1:B:1148:SER:HG	1:B:1183:ARG:HD3	1.74	0.52
1:B:801:GLU:N	1:B:801:GLU:CD	2.68	0.52
1:A:818:ASN:HD21	1:A:821:SER:CA	2.22	0.52
1:B:729:CYS:HB3	1:B:737:CYS:O	2.09	0.52
1:B:806:LEU:HD23	1:B:841:ILE:HD11	1.92	0.52
1:B:1058:TYR:O	1:B:1061:ILE:HG13	2.09	0.52
1:B:1192:GLN:O	1:B:1195:PHE:HB3	2.10	0.52
1:B:848:LEU:HD23	1:B:852:ASN:HA	1.92	0.52
1:A:599:GLU:OE2	1:A:600:LYS:O	2.28	0.52
1:B:661:ILE:HG13	1:B:830:ALA:HB1	1.92	0.52
1:A:929:TYR:O	1:A:932:TRP:N	2.29	0.52
1:A:1101:SER:O	1:A:1103:GLU:N	2.42	0.52
1:B:765:PRO:HG2	1:B:1001:TYR:CZ	2.45	0.52
1:B:921:ALA:HB1	1:B:925:ARG:HH12	1.75	0.52
1:A:794:TRP:CE2	1:A:834:ARG:HG2	2.45	0.51
1:B:772:LEU:N	1:B:772:LEU:HD12	2.25	0.51
1:B:1022:TRP:CE3	1:B:1025:ILE:HD11	2.46	0.51
1:A:772:LEU:HD12	1:A:772:LEU:N	2.25	0.51
1:B:741:TRP:HD1	1:B:742:PRO:O	1.92	0.51
1:B:796:ASP:O	1:B:797:HIS:HB2	2.10	0.51
1:B:653:GLN:HA	1:B:653:GLN:OE1	2.10	0.51
1:B:787:THR:HG21	1:B:816:PHE:CD2	2.44	0.51
1:A:692:LYS:O	1:A:693:GLU:C	2.52	0.51
1:B:741:TRP:HB2	1:B:742:PRO:HD2	1.93	0.51
1:B:910:ARG:O	1:B:910:ARG:HG3	2.11	0.51
1:A:689:ASP:H	1:A:866:GLN:HE22	1.58	0.51
1:A:904:LEU:HD13	1:A:1197:TYR:CD1	2.45	0.51
1:B:1065:LEU:HA	1:B:1079:PHE:HA	1.93	0.51
1:A:828:SER:HB3	1:A:835:THR:HG22	1.91	0.51
1:A:637:ARG:HD2	1:A:869:LEU:CD1	2.41	0.51
1:A:1107:ALA:HB1	1:A:1108:GLU:OE2	2.11	0.51
1:A:1171:ASP:O	1:A:1175:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1192:GLN:O	1:A:1195:PHE:HB3	2.10	0.51
1:A:996:SER:CB	1:A:1183:ARG:HE	2.24	0.51
1:A:1014:LEU:C	1:A:1016:GLU:N	2.67	0.51
1:A:953:ILE:HG23	1:A:954:PRO:HD2	1.93	0.50
1:A:1065:LEU:HA	1:A:1079:PHE:HA	1.93	0.50
1:B:649:LYS:HB3	1:B:650:PRO:HD2	1.93	0.50
1:B:856:VAL:O	1:B:857:TYR:C	2.54	0.50
1:A:1029:LYS:HA	1:A:1090:ARG:NH2	2.26	0.50
1:A:929:TYR:O	1:A:932:TRP:HB2	2.11	0.50
1:A:962:LEU:O	1:A:962:LEU:HD23	2.11	0.50
1:B:929:TYR:HB3	1:B:932:TRP:CG	2.46	0.50
1:B:1049:GLN:C	1:B:1051:TRP:H	2.19	0.50
1:A:602:LEU:H	1:A:602:LEU:CD2	2.25	0.50
1:A:661:ILE:HG13	1:A:830:ALA:HB1	1.94	0.50
1:A:1023:GLN:HB3	1:A:1027:GLN:HE21	1.76	0.50
1:A:1063:VAL:HG12	1:A:1081:LEU:HD22	1.94	0.50
1:A:893:THR:O	1:A:1171:ASP:CG	2.54	0.50
1:B:697:TYR:CE1	1:B:839:ILE:HG23	2.47	0.50
1:B:904:LEU:HD13	1:B:1197:TYR:CD1	2.46	0.50
1:B:942:GLU:HG2	1:B:943:ASN:HD22	1.72	0.50
1:B:1107:ALA:HB1	1:B:1108:GLU:OE2	2.11	0.50
1:B:755:VAL:O	1:B:774:ILE:HA	2.11	0.50
1:B:1101:SER:C	1:B:1103:GLU:N	2.64	0.50
1:B:1171:ASP:O	1:B:1175:VAL:HG23	2.12	0.50
1:A:897:LEU:CD1	1:A:1168:GLU:HA	2.35	0.50
1:A:995:ALA:CB	1:A:1010:ALA:HB2	2.42	0.50
1:A:1018:ILE:HD11	1:A:1048:ALA:CB	2.38	0.50
1:A:1039:LEU:HD22	1:A:1049:GLN:HG3	1.92	0.50
1:B:962:LEU:HD12	1:B:992:TYR:N	2.27	0.50
1:A:743:SER:C	1:A:745:GLU:N	2.69	0.50
1:B:841:ILE:HG22	1:B:845:LEU:CD1	2.42	0.50
1:A:951:ASN:ND2	1:A:951:ASN:H	2.10	0.50
1:B:743:SER:C	1:B:745:GLU:N	2.69	0.50
1:B:911:ASP:HB2	1:B:912:PRO:CD	2.28	0.50
1:B:993:ILE:HG13	1:B:994:ASN:H	1.77	0.50
1:B:629:LEU:O	1:B:629:LEU:HD13	2.12	0.49
1:B:651:PHE:O	1:B:652:ASN:ND2	2.43	0.49
1:B:928:SER:C	1:B:930:ARG:H	2.19	0.49
1:B:933:ARG:CG	1:B:934:THR:N	2.74	0.49
1:B:1172:ILE:O	1:B:1176:VAL:HG23	2.12	0.49
1:A:848:LEU:C	1:A:850:ALA:N	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:942:GLU:HG2	1:A:943:ASN:HD22	1.77	0.49
1:A:1083:HIS:ND1	1:A:1083:HIS:N	2.60	0.49
1:B:851:GLU:HB3	1:B:853:LYS:HE2	1.95	0.49
1:A:1058:TYR:HB2	1:A:1061:ILE:HD11	1.95	0.49
1:A:832:VAL:HG23	1:A:833:GLY:N	2.28	0.49
1:B:767:TYR:HA	1:B:790:GLN:O	2.12	0.49
1:B:848:LEU:C	1:B:850:ALA:N	2.70	0.49
2:D:2002:GLU:C	2:D:2003:GLU:HG3	2.36	0.49
1:A:941:GLU:OE1	1:A:941:GLU:HA	2.13	0.49
1:A:1099:ASN:O	1:A:1100:TRP:HB2	2.13	0.49
1:B:832:VAL:HG23	1:B:833:GLY:N	2.27	0.49
1:B:929:TYR:O	1:B:930:ARG:C	2.54	0.49
1:B:938:GLY:HA2	1:B:992:TYR:CE1	2.48	0.49
1:A:728:ARG:HG2	1:A:792:THR:HG22	1.94	0.49
1:A:1102:VAL:HG11	1:A:1145:ARG:NE	2.28	0.49
1:B:929:TYR:O	1:B:932:TRP:N	2.31	0.49
1:A:637:ARG:HD2	1:A:869:LEU:HD13	1.93	0.49
1:A:1126:LYS:O	1:A:1127:ASN:HB2	2.12	0.49
1:B:901:HIS:N	1:B:902:PRO:CD	2.75	0.49
1:B:1002:TRP:HZ2	1:B:1166:THR:HG21	1.78	0.49
1:A:691:PHE:O	1:A:692:LYS:HG3	2.12	0.49
1:A:1008:ILE:HB	1:A:1141:LEU:HG	1.95	0.49
1:A:1065:LEU:HD23	1:A:1065:LEU:O	2.12	0.49
1:A:1107:ALA:CB	1:A:1108:GLU:OE2	2.61	0.49
1:B:602:LEU:N	1:B:602:LEU:HD13	2.27	0.49
1:B:1041:HIS:ND1	1:B:1041:HIS:C	2.71	0.49
1:A:1101:SER:C	1:A:1103:GLU:N	2.71	0.49
1:B:617:TYR:CE2	1:B:621:ILE:HD13	2.47	0.49
1:B:638:VAL:HG12	1:B:639:PHE:N	2.26	0.49
1:A:949:ASN:HD22	1:A:949:ASN:C	2.19	0.48
1:B:618:LYS:O	1:B:621:ILE:HG13	2.13	0.48
1:B:1000:SER:O	1:B:1001:TYR:C	2.56	0.48
1:A:622:ALA:O	1:A:623:ASP:CG	2.56	0.48
1:B:799:VAL:HB	1:B:879:LEU:HD12	1.95	0.48
1:B:942:GLU:OE1	1:B:942:GLU:N	2.43	0.48
1:B:947:ASN:C	1:B:949:ASN:N	2.70	0.48
1:A:998:ILE:O	1:A:1006:VAL:HG13	2.12	0.48
1:B:851:GLU:OE1	1:B:853:LYS:HE3	2.12	0.48
1:B:867:ARG:HG2	1:B:870:MSE:HG2	1.96	0.48
1:A:796:ASP:O	1:A:797:HIS:HB2	2.13	0.48
1:A:897:LEU:HD12	1:A:1168:GLU:CA	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:ASP:C	1:B:677:ASP:OD2	2.55	0.48
1:B:1028:ARG:HG3	1:B:1028:ARG:HH11	1.78	0.48
1:A:928:SER:C	1:A:930:ARG:H	2.19	0.48
1:B:794:TRP:CE2	1:B:834:ARG:HG2	2.49	0.48
1:B:938:GLY:O	1:B:953:ILE:HD13	2.13	0.48
1:B:1063:VAL:HA	1:B:1081:LEU:CD2	2.44	0.48
1:B:1157:LEU:HD21	1:B:1199:VAL:HG21	1.96	0.48
1:B:713:ARG:O	1:B:717:GLU:HG3	2.14	0.48
1:B:1049:GLN:O	1:B:1051:TRP:N	2.46	0.48
1:A:653:GLN:OE1	1:A:653:GLN:HA	2.13	0.48
1:A:848:LEU:HD23	1:A:852:ASN:HA	1.95	0.48
1:B:691:PHE:O	1:B:692:LYS:HG3	2.14	0.48
1:B:894:GLU:O	1:B:894:GLU:HG2	2.12	0.48
1:B:947:ASN:OD1	1:B:953:ILE:HG12	2.13	0.48
1:A:614:LEU:O	1:A:618:LYS:HG2	2.14	0.48
1:A:844:MSE:HE1	1:A:855:ASP:H	1.75	0.48
1:A:1039:LEU:HD13	1:A:1049:GLN:NE2	2.28	0.48
1:B:844:MSE:HE1	1:B:854:VAL:C	2.37	0.48
1:B:1029:LYS:HA	1:B:1090:ARG:NH2	2.29	0.48
1:A:1049:GLN:C	1:A:1051:TRP:H	2.22	0.48
1:A:887:TYR:O	1:A:891:GLY:HA2	2.14	0.47
1:B:912:PRO:CB	1:B:915:GLU:OE2	2.62	0.47
1:A:806:LEU:HD23	1:A:841:ILE:CD1	2.43	0.47
1:A:947:ASN:C	1:A:949:ASN:N	2.72	0.47
1:B:1039:LEU:HD13	1:B:1049:GLN:HE21	1.79	0.47
1:A:910:ARG:HD2	1:A:915:GLU:O	2.14	0.47
1:A:917:SER:OG	1:A:920:GLU:HG3	2.14	0.47
1:B:611:ASP:O	1:B:613:LEU:N	2.48	0.47
1:B:844:MSE:HE1	1:B:855:ASP:H	1.74	0.47
1:B:911:ASP:CB	1:B:912:PRO:HD3	2.32	0.47
1:A:895:VAL:CG2	1:A:896:ASN:N	2.76	0.47
1:A:929:TYR:O	1:A:930:ARG:C	2.57	0.47
1:A:949:ASN:HD22	1:A:950:SER:N	2.11	0.47
1:A:1028:ARG:HH12	1:A:1136:LYS:HB2	1.80	0.47
1:B:615:GLU:O	1:B:616:THR:C	2.58	0.47
1:B:617:TYR:CZ	1:B:621:ILE:HD13	2.49	0.47
1:B:839:ILE:HD12	1:B:870:MSE:HE1	1.97	0.47
1:B:935:GLN:HB3	1:B:955:TYR:HA	1.96	0.47
1:B:1020:ASP:O	1:B:1023:GLN:HB2	2.14	0.47
1:B:1058:TYR:CD1	1:B:1058:TYR:N	2.81	0.47
1:A:617:TYR:CZ	1:A:621:ILE:HD13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:903:TYR:O	1:B:907:MSE:HB2	2.15	0.47
1:A:884:LEU:O	1:A:888:ASN:HB2	2.14	0.47
1:A:924:GLN:NE2	1:A:924:GLN:HA	2.30	0.47
1:A:962:LEU:HB3	1:A:991:LYS:HB3	1.95	0.47
1:B:689:ASP:H	1:B:866:GLN:NE2	2.12	0.47
1:B:845:LEU:O	1:B:849:GLU:HG3	2.14	0.47
1:B:929:TYR:CE2	1:B:1181:LYS:NZ	2.81	0.47
1:B:946:LYS:C	1:B:947:ASN:HD22	2.22	0.47
1:B:1082:ARG:HB3	1:B:1082:ARG:HH11	1.79	0.47
1:A:648:ARG:HG3	1:A:648:ARG:HH11	1.79	0.47
1:A:713:ARG:O	1:A:717:GLU:HG3	2.15	0.47
1:B:658:TYR:CG	2:D:2004:PTR:HB2	2.50	0.47
1:A:851:GLU:HB2	1:A:853:LYS:HG2	1.97	0.47
1:B:929:TYR:CD2	1:B:1181:LYS:HG3	2.50	0.47
1:B:1142:ILE:HD13	1:B:1154:PHE:CD2	2.39	0.47
1:B:601:GLN:C	1:B:602:LEU:HD13	2.41	0.47
1:B:1039:LEU:HD13	1:B:1049:GLN:NE2	2.30	0.47
1:A:732:GLY:O	1:A:733:ASN:HB2	2.14	0.46
1:A:932:TRP:CH2	1:A:933:ARG:NH2	2.83	0.46
1:B:897:LEU:HG	1:B:1168:GLU:O	2.15	0.46
1:B:1088:ASP:O	1:B:1089:SER:CB	2.57	0.46
1:A:611:ASP:O	1:A:613:LEU:N	2.48	0.46
1:B:1187:VAL:O	1:B:1187:VAL:HG12	2.15	0.46
1:A:1184:LEU:HD22	1:A:1184:LEU:HA	1.75	0.46
1:B:1203:THR:O	1:B:1204:TYR:CD1	2.69	0.46
1:A:615:GLU:CD	1:A:615:GLU:H	2.23	0.46
1:A:844:MSE:HE2	1:A:856:VAL:CA	2.45	0.46
1:A:901:HIS:N	1:A:902:PRO:CD	2.78	0.46
1:B:914:SER:O	1:B:915:GLU:C	2.58	0.46
1:A:871:VAL:O	1:A:871:VAL:HG12	2.15	0.46
1:A:1142:ILE:HD13	1:A:1154:PHE:CD2	2.40	0.46
1:B:872:GLN:HG3	1:B:873:VAL:HG23	1.97	0.46
1:B:1102:VAL:HG11	1:B:1145:ARG:HE	1.80	0.46
1:A:855:ASP:OD2	1:A:858:GLY:HA3	2.15	0.46
1:A:913:PRO:C	1:A:915:GLU:N	2.73	0.46
1:A:1083:HIS:CG	1:A:1085:LYS:HB3	2.50	0.46
1:B:928:SER:O	1:B:930:ARG:N	2.38	0.46
1:B:895:VAL:HG22	1:B:896:ASN:O	2.15	0.46
1:B:1007:MSE:HE2	1:B:1155:CYS:SG	2.56	0.46
1:B:957:TYR:O	1:B:957:TYR:CD1	2.69	0.46
1:B:1017:THR:O	1:B:1019:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1156:ALA:O	1:B:1157:LEU:C	2.59	0.46
1:A:672:SER:HB2	1:A:717:GLU:OE2	2.16	0.46
1:B:608:ILE:O	1:B:853:LYS:HA	2.16	0.46
1:B:787:THR:HG21	1:B:816:PHE:CE2	2.51	0.46
1:B:894:GLU:HG2	1:B:1169:VAL:CG2	2.45	0.46
1:B:1065:LEU:O	1:B:1065:LEU:HD23	2.15	0.46
1:A:937:ILE:HG12	1:A:956:ASP:OD1	2.16	0.46
1:B:605:VAL:CG2	1:B:857:TYR:HB3	2.44	0.46
1:B:1100:TRP:CH2	1:B:1150:GLN:HB2	2.51	0.46
1:A:1000:SER:O	1:A:1001:TYR:C	2.56	0.45
1:A:1157:LEU:HD21	1:A:1199:VAL:HG21	1.97	0.45
1:B:990:SER:O	1:B:991:LYS:HD3	2.15	0.45
1:B:1205:PRO:C	1:B:1207:GLN:H	2.24	0.45
1:A:629:LEU:O	1:A:629:LEU:HD13	2.15	0.45
1:A:1032:VAL:CG2	1:A:1123:LEU:HD23	2.47	0.45
1:B:622:ALA:O	1:B:623:ASP:CG	2.59	0.45
1:B:764:CYS:HB3	1:B:765:PRO:CD	2.45	0.45
1:B:859:TYR:O	1:B:863:LEU:HG	2.16	0.45
1:B:894:GLU:HG2	1:B:1169:VAL:HG22	1.97	0.45
1:B:1087:LYS:HE3	1:B:1087:LYS:CA	2.47	0.45
1:B:912:PRO:HA	1:B:913:PRO:HD2	1.57	0.45
1:A:806:LEU:O	1:A:809:LEU:HD23	2.17	0.45
1:A:960:VAL:HG22	1:A:997:PHE:CE2	2.50	0.45
1:B:1017:THR:C	1:B:1019:GLY:N	2.74	0.45
1:A:839:ILE:O	1:A:840:GLY:C	2.59	0.45
1:B:1117:GLN:HE21	1:B:1117:GLN:HB3	1.61	0.45
1:A:845:LEU:O	1:A:849:GLU:HG3	2.16	0.45
1:A:937:ILE:HG21	1:A:959:ARG:CD	2.47	0.45
1:A:1039:LEU:HD13	1:A:1049:GLN:HE21	1.82	0.45
1:A:1049:GLN:O	1:A:1051:TRP:N	2.49	0.45
1:B:637:ARG:HD2	1:B:869:LEU:CD1	2.46	0.45
1:B:748:THR:OG1	1:B:757:LYS:HB2	2.16	0.45
1:B:959:ARG:O	1:B:959:ARG:HG3	2.17	0.45
1:A:638:VAL:HG12	1:A:639:PHE:N	2.24	0.45
1:A:658:TYR:CG	2:C:2004:PTR:HB2	2.52	0.45
1:B:1014:LEU:HD23	1:B:1014:LEU:HA	1.81	0.45
1:A:873:VAL:HB	1:A:876:GLN:HG3	1.99	0.45
1:B:671:LEU:HD11	1:B:683:ILE:HB	1.99	0.45
1:B:778:LYS:O	1:B:778:LYS:HD3	2.17	0.45
1:B:1082:ARG:CD	1:B:1086:ARG:HA	2.46	0.45
1:B:1160:LEU:HD13	1:B:1172:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:ILE:CG1	1:A:816:PHE:HE2	2.29	0.44
1:A:938:GLY:O	1:A:953:ILE:HD13	2.17	0.44
1:A:1093:TYR:N	1:A:1093:TYR:CD1	2.86	0.44
1:A:743:SER:OG	1:A:746:GLU:CG	2.62	0.44
1:A:874:GLU:O	1:A:878:ILE:HG13	2.18	0.44
1:B:763:ARG:HB3	1:B:763:ARG:HH11	1.82	0.44
1:B:953:ILE:HG23	1:B:954:PRO:HD2	1.98	0.44
1:B:1013:PRO:HG3	1:B:1050:TYR:CD2	2.52	0.44
1:B:856:VAL:O	1:B:860:VAL:HG23	2.18	0.44
1:A:618:LYS:O	1:A:621:ILE:HG13	2.17	0.44
1:A:691:PHE:CZ	1:A:847:GLY:HA2	2.52	0.44
1:A:755:VAL:O	1:A:774:ILE:HA	2.17	0.44
1:A:863:LEU:HD22	1:A:870:MSE:CE	2.45	0.44
1:A:929:TYR:HE2	1:A:1181:LYS:HZ2	1.63	0.44
1:B:783:GLY:C	1:B:784:ARG:HG2	2.42	0.44
1:B:929:TYR:O	1:B:932:TRP:HB2	2.17	0.44
1:B:839:ILE:O	1:B:840:GLY:C	2.59	0.44
1:B:1107:ALA:CB	1:B:1108:GLU:OE2	2.65	0.44
1:A:608:ILE:O	1:A:853:LYS:HA	2.18	0.44
1:A:689:ASP:H	1:A:866:GLN:NE2	2.16	0.44
1:A:1041:HIS:O	1:A:1043:ASP:N	2.50	0.44
1:B:621:ILE:HG23	1:B:628:PHE:HE2	1.81	0.44
1:B:949:ASN:HD22	1:B:950:SER:N	2.16	0.44
1:B:962:LEU:CD1	1:B:991:LYS:HB2	2.28	0.44
1:B:1023:GLN:HB3	1:B:1027:GLN:HE21	1.83	0.44
1:B:1025:ILE:HA	1:B:1030:VAL:HG23	1.99	0.44
1:B:1061:ILE:C	1:B:1061:ILE:CD1	2.89	0.44
1:B:1179:LEU:C	1:B:1181:LYS:N	2.73	0.44
1:A:932:TRP:CZ3	1:A:957:TYR:CE2	3.04	0.44
1:A:1055:LYS:O	1:A:1056:GLN:C	2.59	0.44
1:B:1194:GLN:HE21	1:B:1194:GLN:HB3	1.62	0.44
1:A:745:GLU:C	1:A:747:GLY:N	2.74	0.44
1:A:1000:SER:HB3	1:A:1005:GLU:O	2.18	0.44
1:A:1020:ASP:O	1:A:1023:GLN:HB2	2.18	0.44
1:A:1043:ASP:OD1	1:A:1044:GLN:NE2	2.51	0.44
1:A:1050:TYR:H	1:A:1050:TYR:HD2	1.63	0.44
1:A:1063:VAL:HA	1:A:1081:LEU:CD2	2.47	0.44
1:B:960:VAL:HG13	1:B:997:PHE:CE2	2.51	0.44
1:B:1153:ILE:HD11	1:B:1192:GLN:CB	2.45	0.44
2:C:2005:ASP:O	2:C:2006:VAL:HB	2.18	0.44
1:A:1056:GLN:HB3	1:A:1058:TYR:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:768:ILE:O	1:B:768:ILE:HG13	2.16	0.44
1:B:1063:VAL:HG12	1:B:1081:LEU:CD2	2.48	0.44
1:A:872:GLN:HG3	1:A:873:VAL:HG23	2.00	0.43
1:A:1141:LEU:HD23	1:A:1142:ILE:N	2.33	0.43
1:B:801:GLU:CD	1:B:801:GLU:H	2.26	0.43
1:B:813:VAL:CG2	1:B:838:TYR:OH	2.64	0.43
1:B:926:LEU:HG	1:B:1173:PHE:CZ	2.53	0.43
1:B:938:GLY:HA2	1:B:992:TYR:CZ	2.53	0.43
1:B:943:ASN:HA	1:B:946:LYS:HG3	2.00	0.43
1:A:699:ALA:O	1:A:867:ARG:NH1	2.51	0.43
1:A:841:ILE:HG22	1:A:845:LEU:HD11	2.00	0.43
1:B:644:ILE:HG12	1:B:664:TYR:HA	1.99	0.43
1:B:778:LYS:C	1:B:780:LYS:H	2.26	0.43
1:B:1103:GLU:O	1:B:1104:GLN:C	2.61	0.43
1:A:621:ILE:HG23	1:A:628:PHE:HE2	1.82	0.43
1:A:894:GLU:O	1:A:894:GLU:HG2	2.18	0.43
1:A:991:LYS:HG2	1:A:992:TYR:N	2.33	0.43
1:A:1017:THR:C	1:A:1019:GLY:N	2.75	0.43
1:A:1088:ASP:O	1:A:1089:SER:CB	2.58	0.43
1:B:608:ILE:HG21	1:B:613:LEU:HA	2.00	0.43
1:B:644:ILE:HG22	1:B:644:ILE:O	2.18	0.43
1:A:743:SER:C	1:A:745:GLU:H	2.26	0.43
1:A:963:LYS:HB2	1:A:1027:GLN:OE1	2.18	0.43
1:B:912:PRO:HB2	1:B:915:GLU:OE2	2.18	0.43
1:B:1097:TYR:HB2	1:B:1115:MSE:CE	2.40	0.43
1:B:1141:LEU:HD23	1:B:1142:ILE:N	2.33	0.43
1:A:1077:ARG:HE	1:A:1094:GLN:NE2	2.17	0.43
1:B:912:PRO:HB2	1:B:915:GLU:CG	2.49	0.43
1:B:1085:LYS:O	1:B:1086:ARG:O	2.37	0.43
1:A:648:ARG:HG3	1:A:648:ARG:NH1	2.34	0.43
1:A:907:MSE:O	1:A:918:PRO:HD2	2.18	0.43
1:A:959:ARG:NH2	1:A:990:SER:OG	2.51	0.43
1:A:1203:THR:O	1:A:1204:TYR:CD1	2.72	0.43
1:B:650:PRO:C	1:B:652:ASN:H	2.25	0.43
1:B:1041:HIS:O	1:B:1043:ASP:N	2.52	0.43
1:A:608:ILE:HG21	1:A:613:LEU:HA	2.00	0.43
1:A:851:GLU:HB3	1:A:853:LYS:HE2	1.99	0.43
1:A:1017:THR:O	1:A:1019:GLY:N	2.51	0.43
1:B:804:HIS:O	1:B:808:LYS:HB2	2.18	0.43
1:B:948:ARG:O	1:B:948:ARG:HG3	2.18	0.43
1:A:962:LEU:O	1:A:963:LYS:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:LEU:O	1:A:1017:THR:N	2.48	0.43
1:A:1029:LYS:HA	1:A:1090:ARG:HH22	1.82	0.43
1:A:1039:LEU:HD21	1:A:1051:TRP:CH2	2.54	0.43
1:A:1103:GLU:O	1:A:1104:GLN:C	2.61	0.43
1:A:1171:ASP:OD1	1:A:1174:GLN:HB2	2.17	0.43
1:B:699:ALA:O	1:B:867:ARG:NH1	2.51	0.43
1:B:806:LEU:HD12	1:B:806:LEU:HA	1.69	0.43
1:B:962:LEU:HD21	1:B:993:ILE:CG2	2.49	0.43
1:B:1167:GLU:C	1:B:1169:VAL:N	2.77	0.43
1:A:704:ARG:O	1:A:708:VAL:HG13	2.18	0.43
1:A:748:THR:OG1	1:A:757:LYS:HB2	2.18	0.43
1:A:921:ALA:HB1	1:A:925:ARG:HH12	1.84	0.43
1:A:928:SER:O	1:A:930:ARG:N	2.39	0.43
1:A:1030:VAL:HG21	1:A:1141:LEU:HD12	2.00	0.43
1:B:606:GLU:O	1:B:607:PRO:C	2.61	0.43
1:A:957:TYR:O	1:A:957:TYR:CD1	2.72	0.43
1:A:1084:SER:C	1:A:1086:ARG:H	2.26	0.43
1:A:1087:LYS:HE3	1:A:1087:LYS:CA	2.48	0.43
1:A:1156:ALA:O	1:A:1157:LEU:C	2.60	0.43
1:B:1055:LYS:O	1:B:1056:GLN:C	2.61	0.43
1:B:1084:SER:C	1:B:1086:ARG:H	2.27	0.43
1:A:751:PHE:CD1	1:A:751:PHE:N	2.86	0.42
1:A:895:VAL:C	1:A:896:ASN:HD22	2.27	0.42
1:B:684:ASN:OD1	1:B:867:ARG:NH2	2.52	0.42
1:B:844:MSE:HE2	1:B:856:VAL:HA	2.00	0.42
1:B:1057:THR:HB	1:B:1062:GLU:HG3	2.01	0.42
1:A:764:CYS:HB3	1:A:765:PRO:CD	2.49	0.42
1:A:844:MSE:HE1	1:A:854:VAL:C	2.45	0.42
1:A:1126:LYS:O	1:A:1127:ASN:CB	2.67	0.42
1:B:779:GLU:O	1:B:781:ALA:N	2.52	0.42
1:B:1184:LEU:HD13	1:B:1185:GLY:N	2.34	0.42
1:A:929:TYR:HE2	1:A:1181:LYS:NZ	2.16	0.42
1:B:672:SER:HB2	1:B:717:GLU:OE2	2.18	0.42
1:B:789:ILE:CG1	1:B:816:PHE:HE2	2.32	0.42
1:B:1011:GLN:O	1:B:1012:GLY:C	2.62	0.42
1:A:677:ASP:OD2	1:A:677:ASP:C	2.63	0.42
1:A:1014:LEU:HB2	1:A:1017:THR:OG1	2.19	0.42
1:B:704:ARG:HE	1:B:704:ARG:HB3	1.67	0.42
1:B:728:ARG:HG2	1:B:792:THR:HG22	2.00	0.42
1:B:743:SER:C	1:B:745:GLU:H	2.26	0.42
1:B:932:TRP:CH2	1:B:933:ARG:NH2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:937:ILE:HG21	1:B:959:ARG:CD	2.49	0.42
1:B:949:ASN:HD22	1:B:949:ASN:C	2.27	0.42
1:B:1093:TYR:N	1:B:1093:TYR:CD1	2.87	0.42
1:B:1100:TRP:CD2	1:B:1106:PRO:HG3	2.54	0.42
2:D:2002:GLU:HG3	2:D:2003:GLU:N	2.35	0.42
1:A:935:GLN:HB3	1:A:955:TYR:HA	2.01	0.42
1:B:621:ILE:HG23	1:B:628:PHE:CE2	2.55	0.42
1:B:641:LYS:O	1:B:643:PRO:HD3	2.19	0.42
1:A:641:LYS:O	1:A:643:PRO:HD3	2.20	0.42
1:B:806:LEU:HD23	1:B:841:ILE:CD1	2.49	0.42
1:B:906:ASN:O	1:B:908:LYS:N	2.51	0.42
1:B:1058:TYR:HB2	1:B:1061:ILE:HD11	2.02	0.42
1:A:745:GLU:O	1:A:746:GLU:C	2.62	0.42
1:A:947:ASN:ND2	1:A:994:ASN:HD22	2.18	0.42
1:A:1179:LEU:C	1:A:1181:LYS:N	2.76	0.42
1:B:611:ASP:C	1:B:613:LEU:H	2.27	0.42
1:B:796:ASP:C	1:B:798:GLY:H	2.28	0.42
1:B:1064:ASP:OD2	1:B:1066:LYS:HE2	2.20	0.42
1:A:621:ILE:HG23	1:A:628:PHE:CE2	2.54	0.42
1:A:854:VAL:HG23	1:A:854:VAL:O	2.19	0.42
1:A:896:ASN:N	1:A:896:ASN:HD22	2.17	0.42
1:A:997:PHE:HD1	1:A:1006:VAL:HG11	1.85	0.42
1:B:1105:LEU:HD13	1:B:1195:PHE:HB2	2.01	0.42
1:A:697:TYR:CE1	1:A:839:ILE:HG23	2.55	0.42
1:A:763:ARG:HH11	1:A:763:ARG:HB3	1.85	0.42
1:B:877:TYR:O	1:B:881:HIS:HD2	2.01	0.42
1:B:1191:GLU:CD	1:B:1191:GLU:H	2.28	0.42
1:A:799:VAL:HB	1:A:879:LEU:HD12	2.01	0.41
1:B:908:LYS:O	1:B:917:SER:HB2	2.20	0.41
1:B:1105:LEU:HD13	1:B:1195:PHE:CD1	2.54	0.41
1:A:657:ARG:NH1	1:A:703:PRO:O	2.53	0.41
1:A:903:TYR:O	1:A:907:MSE:HB2	2.20	0.41
1:B:784:ARG:HD2	1:B:820:PHE:CE1	2.55	0.41
1:A:804:HIS:O	1:A:808:LYS:HB2	2.21	0.41
1:A:920:GLU:HG2	1:A:1190:PHE:CE2	2.54	0.41
1:A:949:ASN:C	1:A:949:ASN:ND2	2.78	0.41
1:B:602:LEU:HD22	1:B:602:LEU:N	2.33	0.41
1:B:745:GLU:O	1:B:746:GLU:C	2.64	0.41
1:B:1028:ARG:HH12	1:B:1136:LYS:HB2	1.85	0.41
1:A:704:ARG:HE	1:A:704:ARG:HB3	1.67	0.41
1:A:768:ILE:HG12	1:A:790:GLN:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:ARG:O	1:A:961:PRO:HD3	2.21	0.41
1:A:1100:TRP:CD2	1:A:1106:PRO:HG3	2.56	0.41
1:A:1105:LEU:HD13	1:A:1195:PHE:HB2	2.01	0.41
1:A:1144:CYS:O	1:A:1145:ARG:C	2.62	0.41
1:B:791:PHE:CD2	1:B:794:TRP:HB2	2.56	0.41
1:B:1112:LEU:O	1:B:1115:MSE:HB2	2.21	0.41
1:B:1179:LEU:O	1:B:1180:ARG:C	2.62	0.41
1:A:651:PHE:CD1	1:A:651:PHE:N	2.88	0.41
1:A:1001:TYR:CE1	1:A:1163:SER:HB2	2.55	0.41
1:A:1116:ILE:O	1:A:1120:LYS:HB2	2.20	0.41
1:B:1144:CYS:O	1:B:1145:ARG:C	2.62	0.41
1:A:615:GLU:O	1:A:616:THR:C	2.62	0.41
1:A:631:GLU:O	1:A:857:TYR:CE1	2.61	0.41
1:B:910:ARG:HB2	1:B:915:GLU:O	2.20	0.41
1:B:1101:SER:HB3	1:B:1103:GLU:OE2	2.20	0.41
1:B:1171:ASP:CG	1:B:1174:GLN:HB2	2.46	0.41
1:B:863:LEU:C	1:B:865:ARG:N	2.79	0.41
1:B:935:GLN:NE2	1:B:953:ILE:O	2.54	0.41
1:B:1049:GLN:C	1:B:1051:TRP:N	2.79	0.41
1:A:1040:LYS:HB2	1:A:1044:GLN:O	2.21	0.41
1:A:1077:ARG:NE	1:A:1094:GLN:HE22	2.19	0.41
1:B:1108:GLU:HG2	1:B:1111:GLU:CD	2.46	0.41
1:B:1109:PRO:O	1:B:1112:LEU:N	2.53	0.41
1:A:671:LEU:HD11	1:A:683:ILE:HB	2.02	0.41
1:A:801:GLU:CD	1:A:801:GLU:N	2.79	0.41
1:A:893:THR:O	1:A:1171:ASP:OD2	2.38	0.41
1:A:926:LEU:HA	1:A:927:PRO:HD3	1.96	0.41
1:A:993:ILE:O	1:A:993:ILE:CG2	2.67	0.41
1:A:1011:GLN:O	1:A:1012:GLY:C	2.61	0.41
1:B:730:GLU:OE1	1:B:735:ASN:HA	2.20	0.41
1:B:789:ILE:HD12	1:B:813:VAL:HG12	2.00	0.41
1:B:917:SER:OG	1:B:920:GLU:HG3	2.21	0.41
1:B:929:TYR:HE2	1:B:1181:LYS:HZ2	1.54	0.41
1:A:763:ARG:O	1:A:763:ARG:HG2	2.20	0.41
1:A:943:ASN:ND2	1:A:943:ASN:N	2.68	0.41
1:A:996:SER:HB2	1:A:1183:ARG:HE	1.84	0.41
1:A:1028:ARG:HH12	1:A:1136:LYS:HE3	1.86	0.41
1:A:1171:ASP:CG	1:A:1174:GLN:HB2	2.46	0.41
1:A:856:VAL:O	1:A:860:VAL:HG23	2.21	0.40
1:A:952:VAL:HG12	1:A:952:VAL:O	2.20	0.40
1:A:1047:CYS:SG	1:A:1048:ALA:N	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1180:ARG:HD2	1:A:1186:MSE:O	2.21	0.40
1:B:1083:HIS:CG	1:B:1085:LYS:HB3	2.56	0.40
1:A:802:ASP:O	1:A:803:PRO:C	2.64	0.40
1:A:896:ASN:ND2	1:A:1169:VAL:HG23	2.35	0.40
1:A:1102:VAL:HG11	1:A:1145:ARG:HE	1.86	0.40
1:A:1105:LEU:HD13	1:A:1195:PHE:CD1	2.57	0.40
1:A:1108:GLU:HB2	1:A:1110:LYS:HZ1	1.80	0.40
1:B:648:ARG:HH11	1:B:648:ARG:HG3	1.85	0.40
1:B:926:LEU:HA	1:B:927:PRO:HD3	1.95	0.40
1:B:932:TRP:CZ3	1:B:957:TYR:CE2	3.09	0.40
1:B:1122:LYS:HD3	1:B:1122:LYS:HA	1.92	0.40
1:A:812:ARG:HG2	1:A:812:ARG:NH1	2.35	0.40
1:A:1002:TRP:O	1:A:1005:GLU:HB2	2.22	0.40
1:A:1028:ARG:HG3	1:A:1028:ARG:NH1	2.36	0.40
1:A:1109:PRO:HB3	1:A:1199:VAL:HG12	2.03	0.40
1:B:844:MSE:HE3	1:B:854:VAL:CB	2.31	0.40
1:B:915:GLU:O	1:B:916:PRO:C	2.63	0.40
1:B:810:ARG:NH1	1:B:845:LEU:HD13	2.37	0.40
1:A:869:LEU:HA	1:A:869:LEU:HD12	1.90	0.40
1:A:1017:THR:O	1:A:1018:ILE:C	2.65	0.40
1:A:1199:VAL:HG23	1:A:1200:ILE:N	2.36	0.40
1:B:936:HIS:O	1:B:937:ILE:C	2.64	0.40
1:B:947:ASN:C	1:B:949:ASN:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	568/610 (93%)	457 (80%)	80 (14%)	31 (6%)	1 4
1	B	568/610 (93%)	450 (79%)	84 (15%)	34 (6%)	1 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	3/6 (50%)	2 (67%)	0	1 (33%)	0	0
2	D	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
All	All	1142/1232 (93%)	911 (80%)	165 (14%)	66 (6%)	1	4

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	779	GLU
1	A	929	TYR
1	A	932	TRP
1	A	1015	LYS
1	A	1086	ARG
1	A	1089	SER
1	A	1099	ASN
1	A	1125	GLN
1	B	603	MSE
1	B	780	LYS
1	B	929	TYR
1	B	932	TRP
1	B	1086	ARG
1	B	1089	SER
1	B	1099	ASN
1	B	1188	SER
1	B	1207	GLN
2	C	2002	GLU
1	A	611	ASP
1	A	612	ILE
1	A	677	ASP
1	A	930	ARG
1	A	952	VAL
1	A	1042	GLY
1	A	1050	TYR
1	A	1100	TRP
1	A	1102	VAL
1	A	1107	ALA
1	A	1124	PRO
1	B	611	ASP
1	B	612	ILE
1	B	677	ASP
1	B	930	ARG
1	B	952	VAL

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Mol	Chain	Res	Type
1	B	1015	LYS
1	B	1042	GLY
1	B	1050	TYR
1	B	1100	TRP
1	B	1102	VAL
1	B	1107	ALA
1	A	780	LYS
1	B	672	SER
1	B	833	GLY
1	B	913	PRO
1	B	1156	ALA
1	B	1187	VAL
1	A	610	ALA
1	A	637	ARG
1	A	692	LYS
1	B	692	LYS
1	B	1018	ILE
1	A	902	PRO
1	A	913	PRO
1	A	1048	ALA
1	B	637	ARG
1	B	673	GLU
1	B	902	PRO
1	B	915	GLU
1	B	927	PRO
1	A	800	PRO
1	B	610	ALA
1	B	779	GLU
1	A	1018	ILE
1	A	625	GLY
1	A	833	GLY
1	A	927	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	517/538 (96%)	447 (86%)	70 (14%)	4	12
1	B	516/538 (96%)	449 (87%)	67 (13%)	4	13
2	C	5/5 (100%)	5 (100%)	0	100	100
2	D	5/5 (100%)	4 (80%)	1 (20%)	1	4
All	All	1043/1086 (96%)	905 (87%)	138 (13%)	4	13

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	599	GLU
1	A	602	LEU
1	A	608	ILE
1	A	611	ASP
1	A	612	ILE
1	A	614	LEU
1	A	618	LYS
1	A	629	LEU
1	A	637	ARG
1	A	641	LYS
1	A	648	ARG
1	A	651	PHE
1	A	653	GLN
1	A	674	ILE
1	A	698	ILE
1	A	701	GLN
1	A	757	LYS
1	A	775	VAL
1	A	777	LYS
1	A	784	ARG
1	A	785	GLU
1	A	792	THR
1	A	806	LEU
1	A	813	VAL
1	A	835	THR
1	A	848	LEU
1	A	864	ARG
1	A	874	GLU
1	A	893	THR
1	A	909	LYS
1	A	926	LEU
1	A	929	TYR
1	A	935	GLN

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Mol	Chain	Res	Type
1	A	951	ASN
1	A	957	TYR
1	A	958	ASN
1	A	959	ARG
1	A	963	LYS
1	A	1016	GLU
1	A	1017	THR
1	A	1028	ARG
1	A	1041	HIS
1	A	1044	GLN
1	A	1049	GLN
1	A	1050	TYR
1	A	1065	LEU
1	A	1082	ARG
1	A	1083	HIS
1	A	1087	LYS
1	A	1088	ASP
1	A	1091	THR
1	A	1102	VAL
1	A	1103	GLU
1	A	1104	GLN
1	A	1109	PRO
1	A	1112	LEU
1	A	1115	MSE
1	A	1117	GLN
1	A	1118	VAL
1	A	1122	LYS
1	A	1123	LEU
1	A	1150	GLN
1	A	1157	LEU
1	A	1169	VAL
1	A	1180	ARG
1	A	1184	LEU
1	A	1187	VAL
1	A	1188	SER
1	A	1189	THR
1	A	1194	GLN
1	B	600	LYS
1	B	602	LEU
1	B	608	ILE
1	B	611	ASP
1	B	612	ILE

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Mol	Chain	Res	Type
1	B	614	LEU
1	B	618	LYS
1	B	629	LEU
1	B	637	ARG
1	B	641	LYS
1	B	651	PHE
1	B	653	GLN
1	B	657	ARG
1	B	674	ILE
1	B	698	ILE
1	B	701	GLN
1	B	708	VAL
1	B	746	GLU
1	B	775	VAL
1	B	777	LYS
1	B	778	LYS
1	B	784	ARG
1	B	785	GLU
1	B	792	THR
1	B	806	LEU
1	B	835	THR
1	B	848	LEU
1	B	864	ARG
1	B	874	GLU
1	B	890	PHE
1	B	909	LYS
1	B	915	GLU
1	B	926	LEU
1	B	929	TYR
1	B	935	GLN
1	B	951	ASN
1	B	957	TYR
1	B	958	ASN
1	B	959	ARG
1	B	965	GLU
1	B	1016	GLU
1	B	1017	THR
1	B	1028	ARG
1	B	1041	HIS
1	B	1044	GLN
1	B	1049	GLN
1	B	1050	TYR

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Mol	Chain	Res	Type
1	B	1056	GLN
1	B	1065	LEU
1	B	1082	ARG
1	B	1083	HIS
1	B	1087	LYS
1	B	1088	ASP
1	B	1091	THR
1	B	1102	VAL
1	B	1103	GLU
1	B	1104	GLN
1	B	1112	LEU
1	B	1115	MSE
1	B	1117	GLN
1	B	1122	LYS
1	B	1150	GLN
1	B	1157	LEU
1	B	1180	ARG
1	B	1184	LEU
1	B	1186	MSE
1	B	1194	GLN
2	D	2005	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	652	ASN
1	A	675	ASN
1	A	718	GLN
1	A	770	GLN
1	A	818	ASN
1	A	866	GLN
1	A	876	GLN
1	A	882	GLN
1	A	888	ASN
1	A	889	GLN
1	A	896	ASN
1	A	924	GLN
1	A	935	GLN
1	A	943	ASN
1	A	947	ASN
1	A	949	ASN
1	A	951	ASN

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Mol	Chain	Res	Type
1	A	958	ASN
1	A	1011	GLN
1	A	1044	GLN
1	A	1049	GLN
1	A	1094	GLN
1	A	1117	GLN
1	A	1121	GLN
1	A	1127	ASN
1	A	1150	GLN
1	B	652	ASN
1	B	718	GLN
1	B	770	GLN
1	B	797	HIS
1	B	818	ASN
1	B	876	GLN
1	B	882	GLN
1	B	888	ASN
1	B	905	HIS
1	B	924	GLN
1	B	935	GLN
1	B	943	ASN
1	B	947	ASN
1	B	949	ASN
1	B	951	ASN
1	B	958	ASN
1	B	994	ASN
1	B	1027	GLN
1	B	1044	GLN
1	B	1049	GLN
1	B	1094	GLN
1	B	1117	GLN
1	B	1150	GLN
1	B	1194	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PTR	D	2004	2	15,16,17	1.82	5 (33%)	17,22,24	2.43	5 (29%)
2	PTR	C	2004	2	15,16,17	1.94	6 (40%)	17,22,24	1.43	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	D	2004	2	1/1/2/3	4/10/11/13	0/1/1/1
2	PTR	C	2004	2	1/1/2/3	1/10/11/13	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2004	PTR	P-OH	3.96	1.67	1.59
2	C	2004	PTR	OH-CZ	2.92	1.47	1.40
2	C	2004	PTR	P-O3P	-2.85	1.44	1.54
2	D	2004	PTR	P-O3P	-2.84	1.44	1.54
2	D	2004	PTR	P-OH	2.70	1.64	1.59
2	D	2004	PTR	CE2-CD2	2.69	1.43	1.38
2	D	2004	PTR	OH-CZ	2.56	1.46	1.40
2	D	2004	PTR	CD2-CG	2.44	1.43	1.38
2	C	2004	PTR	P-O2P	-2.37	1.46	1.54
2	C	2004	PTR	CE2-CD2	2.19	1.42	1.38
2	C	2004	PTR	CD2-CG	2.18	1.43	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2004	PTR	P-OH-CZ	5.41	143.16	123.88
2	D	2004	PTR	OH-CZ-CE2	4.50	132.70	119.22
2	D	2004	PTR	OH-CZ-CE1	-4.33	106.24	119.22
2	D	2004	PTR	O3P-P-OH	2.95	114.04	105.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2004	PTR	CE2-CD2-CG	-2.39	117.86	121.00
2	C	2004	PTR	O3P-P-O2P	2.29	116.39	107.80
2	C	2004	PTR	OH-CZ-CE2	2.15	125.67	119.22

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2004	PTR	CA
2	D	2004	PTR	CA

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2004	PTR	C-CA-CB-CG
2	D	2004	PTR	O-C-CA-CB
2	D	2004	PTR	C-CA-CB-CG
2	D	2004	PTR	CA-CB-CG-CD1
2	D	2004	PTR	CA-CB-CG-CD2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2004	PTR	1	0
2	C	2004	PTR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.